

Lifshitz transitions in a heavy-Fermion liquid driven by short-range antiferromagnetic correlations in the two-dimensional Kondo lattice model

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The heavy-Fermion liquid with short-range antiferromagnetic correlations is carefully considered in the two-dimensional Kondo-Heisenberg lattice model. As the ratio of the local Heisenberg superexchange J_H to the Kondo coupling J_K increases, Lifshitz transitions are anticipated, where the topology of the Fermi surface (FS) of the heavy quasiparticles changes from a hole-like circle to four kidney-like pockets centered around (π, π) . In-between these two limiting cases, a first-order quantum phase transition is identified at $J_H/J_K = 0.1055$ where a small circle begins to emerge within the large deformed circle. When $J_H/J_K = 0.1425$, the two deformed circles intersect each other and then decompose into four kidney-like Fermi pockets via a second-order quantum phase transition. As J_H/J_K increases further, the Fermi pockets are shifted along the direction (π, π) to $(\pi/2, \pi/2)$, and the resulting FS is consistent with the FS obtained recently using the quantum Monte Carlo cluster approach to the Kondo lattice system in the presence of the antiferromagnetic order.

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Quantum phase transitions are emergent phenomena observed in many strongly correlated electron systems and has attracted much interest. An electronic transition associated with the change of Fermi surface (FS) topology, the so-called Lifshitz transition[1], can be induced without any spontaneous symmetry breaking and local order parameter. The Lifshitz transition is assumed to be a quantum phase transition at $T = 0$ and it becomes a crossover at finite temperatures. Elucidating the nature of the Lifshitz transition, it seems that the transition manifests itself dramatically[2, 3] only when other degrees of freedom like lattice or spin couple strongly with the electronic states.

Heavy fermion materials have played a particularly important role in the study of quantum critical phenomena. The Kondo lattice model is believed to capture the basic physics of heavy fermions. The model describes a lattice of local spin-1/2 magnetic moments coupled antiferromagnetically to a single band of conduction electrons. The huge mass enhancement of the quasiparticles can be attributed to the coherent superposition of individual Kondo screening clouds, and the resulting metallic state is characterized by a *large* FS with the Luttinger volume containing both conduction electrons and localized moments. Competing with the Kondo singlet formation, the localized spins indirectly interact with each other via magnetic polarization of the conduction electrons – the Ruderman-Kittel-Kasuya-Yosida interaction. Such interaction dominates at low values of the Kondo exchange coupling and is the driving force for the antiferromagnetic (AFM) long-range order quantum phase transitions[4, 5]. In a recent experiment[6] a jump in the Hall coefficient for YbRh_2Si_2 has been observed, and a sudden change in the FS topology from a large FS to a small one was suggested at the magnetic quantum critical point. The nature of this phase transition is currently under hot debate[7–13].

So far most of investigations focus on the possible FS reconstruction around the magnetic quantum critical point. However, we would like to point out that the FS topology

in the paramagnetic heavy-fermion liquid phase may also be drastically changed by the short-range AFM spin correlations between the localized spins, leading to the Lifshitz phase transitions. The nature of such a quantum phase transition has not been thoroughly explored yet. It is well-known that the large- N fermionic approach can be used to treat the Kondo lattice model in the Kondo singlet regime very efficiently, leading to the paramagnetic heavy-Fermion liquid state[14–16]. To consider the effects of the short-range AFM spin correlations, it is more straightforward to explicitly introduce the Heisenberg AFM superexchange J_H between the localized spins to the Kondo lattice system[8, 9, 12, 17, 18].

In this paper, we apply the large- N fermionic approach to the Kondo-Heisenberg model on a two-dimensional square lattice in the limit of $J_K > J_H$. By introducing uniform short-range AFM valence-bond and Kondo screening parameters, a fermionic mean-field theory is carefully re-examined, and such a mean-field theory becomes exact when the degeneracy of the localized spins N becomes infinite. Away from half-filling, at the conduction electron density $n_c = 0.9$, for example, as $x = J_H/J_K$ increases, we find that the topology of the FS of the heavy quasiparticles changes from one hole-like circle to four kidney-like pockets around (π, π) . In-between these two distinct limits, we will identify a first-order quantum phase transition at $x_{1c} = 0.1055$, where a small circle begin to emerge within the large deformed circle. Then the inner circle gradually expands, deforming to a rotated squared circle. When $x_{2c} = 0.1425$, the two deformed circles intersect each other and then decompose into four kidney-like Fermi pockets, resulting in a second-order quantum phase transition.

The model Hamiltonian of the Kondo-Heisenberg lattice model is given by:

$$H = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + J_K \sum_i \mathbf{S}_i \cdot \mathbf{S}_i + J_H \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

where $c_{\mathbf{k}\sigma}^\dagger$ creates a conduction electron on an extended orbital with wave vector \mathbf{k} and z-component of spin $\sigma = \uparrow, \downarrow$.

The spin-1/2 operators of the local magnetic moments have the fermionic representation $\mathbf{S}_i = \frac{1}{2} \sum_{\sigma\sigma'} f_{i\sigma}^\dagger \boldsymbol{\tau}_{\sigma\sigma'} f_{i\sigma'}$ with a local constraint $\sum_{\sigma} f_{i\sigma}^\dagger f_{i\sigma} = 1$, where $\boldsymbol{\tau}$ is the Pauli matrices. Following the large- N fermionic approach,[8, 17] the Kondo spin exchange and Heisenberg superexchange terms can be expressed up to a chemical potential shift as

$$\begin{aligned} \mathbf{S}_i \cdot \mathbf{S}_j &= -\frac{1}{2} \sum_{\sigma\sigma'} f_{i\sigma}^\dagger f_{j\sigma} f_{j\sigma'}^\dagger f_{i\sigma'}, \\ \mathbf{S}_i \cdot \mathbf{S}_j &= -\frac{1}{2} \sum_{\sigma\sigma'} f_{i\sigma}^\dagger c_{j\sigma} c_{j\sigma'}^\dagger f_{i\sigma'}, \end{aligned}$$

then a uniform short-range AFM valence bond and Kondo screening order parameters can be introduced as

$$\chi = -\sum_{\sigma} \langle f_{i\sigma}^\dagger f_{i+l\sigma} \rangle, \quad V = \sum_{\sigma} \langle c_{i\sigma}^\dagger f_{i\sigma} \rangle. \quad (2)$$

Generally speaking, apart from the uniform short-range AFM valence bond state, there are other possible competing states, including various flux phases or plaquette states. However, the stabilization of those states would require the presence of the translational lattice symmetry breaking and/or additional frustrating interactions. Since there is no evidence of translational symmetry breaking in the paramagnetic heavy-fermion liquid states, we will not consider those effects at this stage. Although most heavy fermion systems are three dimensional, as far as the FS topology is concerned, it is conceptually simpler in the model discussion to start with a two-dimensional case of this Kondo-Heisenberg lattice model.

To avoid the incidental degeneracy of the conduction electron band on a square lattice, we choose $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y - \mu$, where t and t' are the first and second nearest neighbor hopping matrix elements, respectively, while μ is the chemical potential, which should be determined self-consistently by the density of the conduction electrons n_c . Under the uniform mean-field approximation, the f-fermions/spinons form a very narrow band with the dispersion $\chi_{\mathbf{k}} = J_H \chi (\cos k_x + \cos k_y) + \lambda$, where λ is the Lagrangian multiplier to be used to impose the local constraint on average.

In general, there are two interesting mean-field phases. One is the uniform short-range AFM ordered phase in the limit of $J_H > J_K$ where $V = 0$ but $\chi \neq 0$. In this phase, the spinons represented by f-fermions are unconfined and have a dispersion $\chi_{\mathbf{k}}$. Another phase is the heavy electron phase with short-range AFM spin correlations in the limit of $J_H < J_K$, where both $V \neq 0$ and $\chi \neq 0$. Actually the former limit has been extensively studied in many previous investigations,[8, 13, 17] but we will focus on the latter limit.

Thus the corresponding mean-field Hamiltonian reads

$$H = \sum_{\mathbf{k}\sigma} \begin{pmatrix} c_{\mathbf{k}\sigma}^\dagger & f_{\mathbf{k}\sigma}^\dagger \end{pmatrix} \begin{pmatrix} \epsilon_{\mathbf{k}} & -\frac{1}{2}J_K V \\ -\frac{1}{2}J_K V & \chi_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\sigma} \\ f_{\mathbf{k}\sigma} \end{pmatrix} + E_0,$$

with $E_0 = N(-\lambda + J_H \chi^2 + J_K V^2/2)$. The quasiparticle excitation spectra can be easily obtained

$$\varepsilon_{\mathbf{k}}^{(\pm)} = \frac{1}{2} [(\epsilon_{\mathbf{k}} + \chi_{\mathbf{k}}) \pm W_{\mathbf{k}}], \quad (3)$$

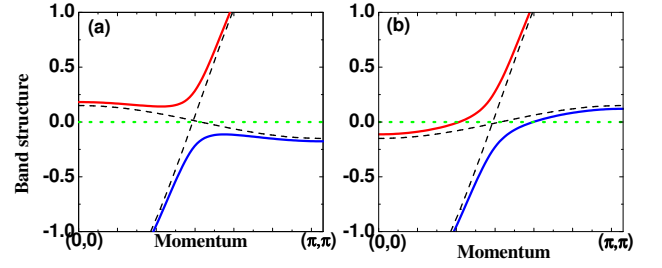


FIG. 1: (Color online) Schematic plot of the conduction electron band $\epsilon_{\mathbf{k}}$ hybridizing with the very narrow band $\chi_{\mathbf{k}}$ in the $n_c = 1$ case. The dashed lines denote the original bands, while the solid lines correspond to the hybridized bands. (a) The short-range AFM order parameter $\chi > 0$, (b) $\chi < 0$. Clear distinction of these two different cases shows that there is always a finite gap in case (a), while being gapless in case (b).

which implies that the conduction electron band $\epsilon_{\mathbf{k}}$ has a finite hybridization with the spinon band $\chi_{\mathbf{k}}$. Here $W_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \chi_{\mathbf{k}})^2 + (J_K V)^2}$. Accordingly, the ground-state energy density can be evaluated as

$$\varepsilon_g = \frac{2}{N} \sum_{\mathbf{k}, \pm} \varepsilon_{\mathbf{k}}^{(\pm)} \theta(-\varepsilon_{\mathbf{k}}^{(\pm)}) - \lambda + J_H \chi^2 + \frac{1}{2} J_K V^2, \quad (4)$$

where $\theta(-\varepsilon)$ is the theta function. Then the self-consistent equations for the mean-field variables χ , V , and λ can be derived by minimizing the ground state energy $\frac{\partial \varepsilon_g}{\partial \chi} = 0$, $\frac{\partial \varepsilon_g}{\partial V} = 0$, $\frac{\partial \varepsilon_g}{\partial \lambda} = 0$, and the chemical potential μ should be deduced from the relation $n_c = -\frac{\partial \varepsilon_g}{\partial \mu}$. This leads to the following self-consistent equations at zero temperature,

$$\begin{aligned} \chi &= -\frac{1}{2N} \sum_{\mathbf{k}, \pm} \theta(-\varepsilon_{\mathbf{k}}^{(\pm)}) \left[1 \mp \frac{(\epsilon_{\mathbf{k}} - \chi_{\mathbf{k}})}{W_{\mathbf{k}}} \right] \gamma_{\mathbf{k}}, \\ 1 &= -\frac{1}{N} \sum_{\mathbf{k}, \pm} \theta(-\varepsilon_{\mathbf{k}}^{(\pm)}) \frac{\pm J_K}{W_{\mathbf{k}}}, \\ 1 &= \frac{1}{N} \sum_{\mathbf{k}, \pm} \theta(-\varepsilon_{\mathbf{k}}^{(\pm)}) \left[1 \mp \frac{(\epsilon_{\mathbf{k}} - \chi_{\mathbf{k}})}{W_{\mathbf{k}}} \right], \\ n_c &= \frac{1}{N} \sum_{\mathbf{k}, \pm} \theta(-\varepsilon_{\mathbf{k}}^{(\pm)}) \left[1 \pm \frac{(\epsilon_{\mathbf{k}} - \chi_{\mathbf{k}})}{W_{\mathbf{k}}} \right], \end{aligned} \quad (5)$$

where $\gamma_{\mathbf{k}} = \cos k_x + \cos k_y$. In the following, we will assume that $t'/t = 0.3$ and $n_c = 0.9$, which is away from half-filling and in the paramagnetic metallic phase.[11]

The most important thing is to notice that the resulting two renormalized quasiparticle bands $\varepsilon_{\mathbf{k}}^{(\pm)}$ crucially depend on the sign of the AFM order parameter χ . If χ is positive, $\varepsilon_{\mathbf{k}}^{(-)}$ and $\varepsilon_{\mathbf{k}}^{(+)}$ are separated by an indirect energy gap as displayed in Fig.1a, where the conduction electrons hybridize with the *hole-like* f-fermions/spinons. For the negative value of χ , however, the renormalized quasiparticle bands $\varepsilon_{\mathbf{k}}^{(-)}$ and $\varepsilon_{\mathbf{k}}^{(+)}$ always have a finite overlap as shown in Fig.1b, where the conduction electrons actually hybridize with the *particle-like*

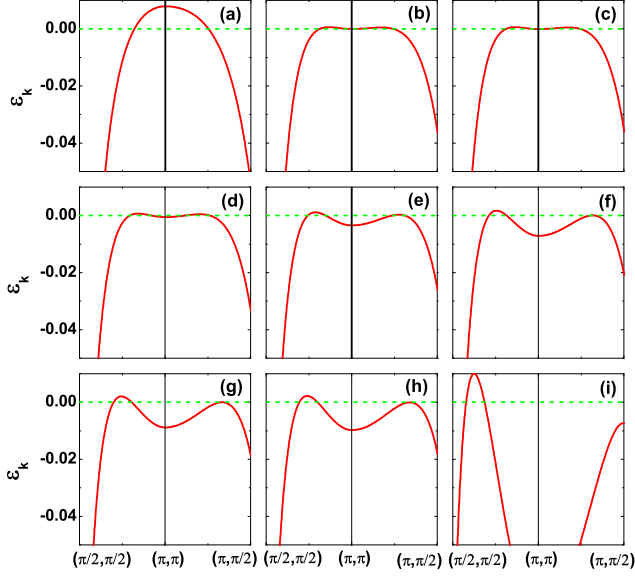


FIG. 2: (Color online) The lower renormalized quasiparticle band in the direction $(\pi/2, \pi/2) \rightarrow (\pi, \pi) \rightarrow (\pi, \pi/2)$ as increasing the strength of the AFM spin fluctuations. (a) to (i) correspond to $J_K/t = 2.0$ and $J_H/J_K = 0.05, 0.1055, 0.1056, 0.11, 0.125, 0.1375, 0.1425, 0.145$, and 0.25 , respectively. In the calculation $t'/t = 0.3$ and $n_c = 0.9$. The dash line denotes the Fermi level.

f-fermions/spinons. Even in the half-filling case $n_c = 1$, the model system has the properties of a semi-metal with a FS consisting of one electron-like pocket around $\mathbf{k} = (0, 0)$ and one hole-like pocket around $\mathbf{k} = (\pi, \pi)$. Then the resulting ground state will exhibit an instability towards the AFM spin-density wave or s_{\pm} -wave pairing superconductivity.[19]

When the self-consistent calculations are carefully performed, we find that the mean-field AFM order parameter χ is *always* positive in the range $0 < J_H/J_K \leq 0.5$ so that the resulting state is a stable paramagnetic metal. In Fig.2, as the strength of the AFM spin fluctuations grows up, we present the evolution of the band structure of the renormalized heavy quasiparticles around the Fermi level in the direction $(\pi/2, \pi/2) \rightarrow (\pi, \pi) \rightarrow (\pi, \pi/2)$ of the first Brillouin zone. Fig.2a to Fig.2i correspond to $J_K/t = 2.0$ and $J_H/J_K = 0.05, 0.1055, 0.1056, 0.11, 0.125, 0.1375, 0.1425, 0.145$, and 0.25 , respectively.

For a fixed J_K/t , we can clearly see in Fig.2a and Fig.2b that the M point (π, π) is the maximum of the lower renormalized quasiparticle band $\varepsilon_{\mathbf{k}}^{(-)}$ for $J_H/J_K < 0.1055$, and then the Fermi level ($\varepsilon_F = 0$) crosses the quasiparticle band only once in the the direction $(\pi/2, \pi/2) \rightarrow (\pi, \pi)$ or $(\pi, \pi) \rightarrow (\pi, \pi/2)$. For $J_H/J_K \geq 0.1055$, the M point becomes a local minimum of the lower renormalized quasiparticle band $\varepsilon_{\mathbf{k}}^{(-)}$ in Fig.2c to Fig.2i. In the direction of $(\pi/2, \pi/2) \rightarrow (\pi, \pi)$, the Fermi level always crosses the quasiparticle band twice. However, in the the direction of $(\pi, \pi) \rightarrow (\pi, \pi/2)$, the Fermi level crosses the quasiparticle band twice only when $0.1055 \leq J_H/J_K < 0.1425$, while the Fermi level can cross the quasiparticle band once for $J_H/J_K \geq 0.1425$. Therefore,

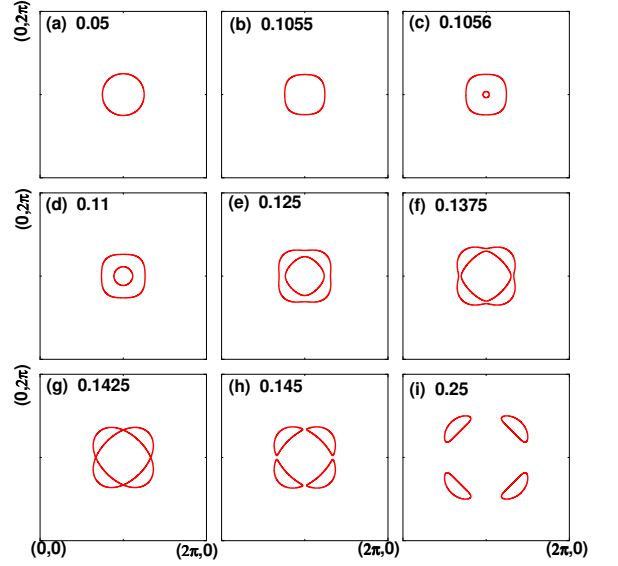


FIG. 3: (Color online) The Fermi surface corresponding to the lower renormalized quasiparticle band shown in Fig.2. The ratio J_H/J_K is indicated in graphs. Here the center of the Fermi surface has been shifted from $(0, 0)$ to (π, π) in order to clearly exhibit the topology of the Fermi surface.

both $J_H/J_K = 0.1055$ and $J_H/J_K = 0.1425$ represent two special coupling strengths.

Once the renormalized quasiparticle band structure is available, the corresponding FS can be easily obtained. Corresponding to the band structure shown in Fig.2, the FS are displayed in Fig.3, where we have shifted the center of the FS from $(0, 0)$ to (π, π) . For a fixed $J_K/t = 2.0$, we can clearly see that the FS is a hole-like circle around (π, π) for the parameter range $0 \leq J_H/t \leq 0.1$, and then the shape of FS deforms to a square for $0.1 < J_H/J_K \leq 0.1055$. At $J_H/J_K = 0.1056$, the topology of the FS starts to change: a small circle emerges in the center of the deformed large square FS. As J_H/J_K is further increased, both circles expand and the small one is deformed into a rotated square. Up to $J_H/J_K = 0.1425$, the two deformed circles intersect each other and then decompose into four kidney-like Fermi pockets. When J_H/J_K continues to increase, the resulting FS (not included here) will be shifted outward along the direction $M \rightarrow \Gamma$.

Recently, a quantum Monte Carlo cluster approach has been proposed to study the evolution of the Fermi surface across the magnetic order-disorder transition in the two-dimensional Kondo lattice system[11]. In the AFM long-range ordered phase, the Kondo screening does not break down, and the heavy fermion bands drop below the FS giving way to hole pockets centered around $\mathbf{k} = (\pi/2, \pi/2)$ and equivalent points. These results are fully consistent with the FS obtained by our calculation in the range $0.25 \leq J_H/J_K < 1$.

In order to study the topology changes of the FS from the quantum phase transition aspects, we calculate the ground

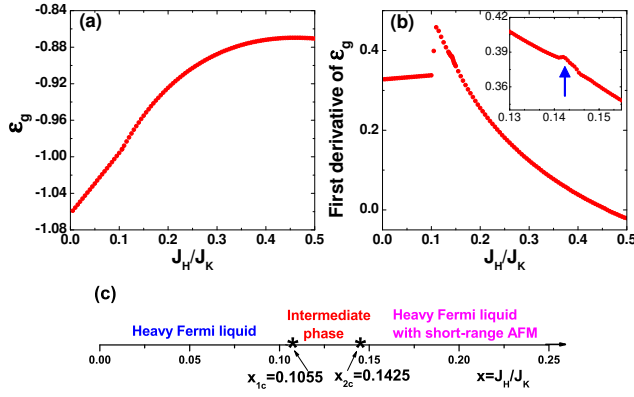


FIG. 4: (Color online) (a) The ground state energy density ε_g as a function of $x = J_H/J_K$. (b) The first-order derivative of ε_g with respect to the parameter x . (c) The ground-state phase diagram of the system.

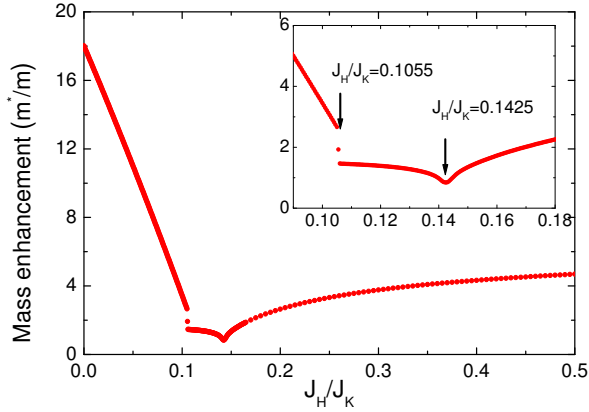


FIG. 5: (Color online) The quasiparticle mass enhancement factor as a function of $x = J_H/J_K$.

state energy density ε_g and its first-order derivative with respect to the ratio of the coupling parameters $x = J_H/J_K$. The numerical results are displayed in Fig.4a and Fig.4b. We find that two non-analytical points appear in the ground state energy density. ε_g is finite and continuous in the parameter range $0 < x < 0.5$. However, its first-order derivative has a large jump at $x_{1c} = 0.1055$, corresponding to a first-order (discontinuous) quantum phase transition. Moreover, a small kink appears at $x_{2c} = 0.1425$ in the first-order derivative, which corresponds to a jump in the second-order derivative of ε_g . So x_{2c} denotes a second-order (continuous) quantum phase transition. Actually both quantum phase transitions belong to the category of Lifshitz phase transitions. The ground state phase

diagram is delineated in Fig.4c, where there exist three different paramagnetic heavy-fermion liquid phases: the conventional heavy-fermion liquid in $x < 0.105$, the heavy-fermion liquid with strong AFM spin fluctuations in $0.1425 < x < 1$, and the intermediate phase $0.105 < x < 0.1425$.

Moreover, the effective mass of the heavy quasiparticle excitations is a function of the band curvature, so the topological changes of the Fermi surface can be reflected in the effective mass, which is related to the non-interacting band mass by the variation $m^* \delta \varepsilon_{\mathbf{k}}^{(-)} = m \delta \epsilon_{\mathbf{k}}$, averaged over all points on the FS. Hence the mass enhancement factor is given by

$$\frac{m^*}{m} = \left\langle \frac{\partial \varepsilon_{\mathbf{k}}^{(-)}}{\partial \epsilon_{\mathbf{k}}} \right\rangle_{FS}^{-1} = \frac{1}{N} \sum_{\mathbf{k}} \left[\frac{\partial \varepsilon_{\mathbf{k}}^{(-)}}{\partial \epsilon_{\mathbf{k}}} \right]^{-1} \delta(\mu - \varepsilon_{\mathbf{k}}^{(-)}), \quad (6)$$

which is displayed in Fig.5. Here we can also observe the two successive quantum phase transitions at $J_H/J_K = 0.1055$ and 0.1425 , respectively, consistent with the results from the analysis of the ground state energy density. Actually, since the effective mass enhancement factor is related to the optical conductivity in infrared spectroscopy measurements, the above Lifshitz phase transitions can be observed experimentally.

In conclusion, we have carefully studied the heavy-fermion liquid state in the two-dimensional Kondo-Heisenberg lattice system. As J_H/J_K grows up, the topology of the quasiparticle FS rapidly changes from one hole-like circle in the conventional heavy-fermion liquid state to four kidney-like pockets centered around (π, π) , which is very close to the FS near the AFM magnetic quantum critical point. Between these two distinct FSs, a first-order quantum phase transition occurs at $J_H/J_K = 0.1055$, where a small circle emerges within the large deformed circle. When $J_H/J_K = 0.1425$, the two deformed circles intersect each other and then decompose into four kidney-like Fermi pockets, and a second-order quantum phase transition takes place. Both quantum phase transitions belong to the category Lifshitz phase transitions.

To some extent our present mean-field theory captures the heavy-fermion liquid physics of the Kondo-Heisenberg lattice systems, especially the Fermi surface evolution of the renormalized heavy quasiparticles as the short-range AFM spin correlations between the localized magnetic moments are gradually increased. In order to put the present results on a more solid ground, further investigations including the gauge fluctuations associated with the mean-field order parameters are certainly needed.

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